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IMPROVED METHODS FOR COMPUTING MASSES FROM NUMERICAL SIMULATIONS*

Andreas S. KRONFELD

Theoretical Physics Group, Fermi National Accelerator Laboratory,
P.O. Box 500, Batavia, IL 60510, USA

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Abstract

An important advance in the computation of hadron and glueball masses has been the introduction of non-local operators. This talk summarizes the critical signal-to-noise ratio of glueball correlation functions in the continuum limit, and discusses the case of ($q\bar{q}$ and qqq) hadrons in the chiral limit. A new strategy for extracting the masses of excited states is outlined and tested. The lessons learned here suggest that gauge-fixed momentum-space operators might be a suitable choice of interpolating operators.

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IMPROVED METHODS FOR COMPUTING MASSES FROM NUMERICAL SIMULATIONS

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An important advance in the computation of hadron and glueball masses has been the introduction of non-local operators. This talk summarizes the critical signal-to-noise ratio of glueball correlation functions in the continuum limit, and discusses the case of ($q\bar{q}$ and qqq) hadrons in the chiral limit. A new strategy for extracting the masses of excited states is outlined and tested. The lessons learned here suggest that gauge-fixed momentum-space operators might be a suitable choice of interpolating operators.

1. INTRODUCTION

In the past few years several schemes for producing non-local glueball[1, 2, 3] and hadron[4] operators have been developed. These operators yield correlation functions which are much less noisy than their counterparts using local operators, and, consequently, more precise mass estimates at fixed statistics. Except for two attempts[5, 6] the improved methods have not yielded an estimate of excited-state masses. If numerical simulations are to become a versatile tool of elementary particle physics, these masses must be computed, not just for the sake of completeness, but also for the identification of resonance parameters.[7]

The usual way to compute excited state masses is a variational calculation with the matrix of correlations of some set of operators. A typical set will be neither complete nor linearly independent, and only a statistical estimate of the matrix is available. Consequently, the number of accessible states M is likely less than the number of sampled operators N. Singular-value decomposition is a method of determining M from the data and also suggests a variational calculation in the space of the M accessible states, instead of te space of N sampled operators.

The presentation is as follows: Sect. 2 reviews how non-local operators solve the critical signal-to-noise problem for glueballs.[8] Sect. 3 discusses a signal-to-noise problem for hadrons in the chiral limit. The refinement of the usual variational calculation is given in sect. 4. Sect. 5 proposes that momentum-space operators (in a fixed gauge) might offer a useful set of operators.

2. SIGNAL-TO-NOISE RATIO FOR GLUEBALLS

Glueball masses are computed from correlation functions of the form

$$C_r(t) = \langle \Phi_r(t)\, \Phi_r(0) \rangle - \langle \Phi_r(t) \rangle \langle \Phi_r(0) \rangle, \qquad (2.1)$$

where Φ_r is a function of the lattice gauge field with support on the time-slice t. The index r denotes the quantum numbers of the state(s) of interest. A numerical simulation has finite statistics, so another important issue is the noise of $C_r(t)$, which is quantified by the statistical dispersion of $\Phi_r(t)\,\Phi_r(0)$:

$$\sigma_r^2(t_1,t_2) = \qquad (2.2)$$
$$\langle (\Phi_r(t_1)\Phi_r(0))(\Phi_r(0)\Phi_r(t_2)) \rangle - C_r(t_1)C_r(t_2).$$

Eq. (2.2) treats correlated fluctuations between time-slices t_1 and t_2. For $t_{1,2}$ large enough for clustering,[8]

$$\sigma_r^2(t_1,t_2) = C_r(|t_1 - t_2|)C_r(0) - C_r(t_1)C_r(t_2). \qquad (2.3)$$

Generally, the first term dominates, and the signal-to-noise ratio is

$$\frac{\text{SIGNAL}}{\text{NOISE}} = \sqrt{N_{\text{conf}}}\,\frac{C_r(t)}{\sigma_r(t,t)} = \sqrt{N_{\text{conf}}}\,\frac{C_r(t)}{C_r(0)}, \qquad (2.4)$$

for glueball correlation functions.

The correlation function $C_r(0)$ can be ultraviolet divergent for too local choices of interpolating operators Φ_r, such as the plaquette, or other small Wilson loops. If $C_r(0)$ diverges as a^{-z}, then

$$\frac{\text{SIGNAL}}{\text{NOISE}} \propto \sqrt{N_{\text{conf}}}\,a^z, \qquad (2.5)$$

so the ensemble size N_{conf} must grow proportionally

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Table 1: Ultraviolet divergence of the noise for various glueball operators.

method[ref.]	z
plaquette, etc.[10]	5
adjoint lines[11]	0
fuzzy loops[1]	1–4
smeared loops[2, 5]	0
inverse Dirac[3, 8]	0–1
momentum space[sect. 5]	0

to a^{-2z}. For $z > 0$ this is an obstacle to computing continuum-limit masses worse than critical slowing down.

The origin of this divergence has been analyzed in detail.[8] For states accessible to two gluons, define $\varphi^{ab}_{\mu\nu}(P|k)$ by

$$e^{i(p_0+q_0)t}(2\pi)^3\delta^{(3)}(\vec{p}+\vec{q}-\vec{P}_r)\varphi^{ab}_{\mu\nu}(p+q|\tfrac{1}{2}(p-q)) = \frac{1}{2}\frac{\delta^2\Phi_r(t)}{\delta A^a_\mu(p)\delta A^b_\nu(q)}\bigg|_{A=0}, \qquad (2.6)$$

where $\vec{P}_r$ is the three-momentum of the representation r. (An analogous analysis is possible for three-gluon states.) The a-dependence of the signal-to-noise ratio is governed by the ultraviolet degree of divergence[9] of $\varphi^{ab}_{\mu\nu}(P|k)$. If that degree is positive (negative) $C_r(0)$ has (does not have) an ultraviolet divergence. Table 1 gives the signal-to-noise-ratio exponent z for various operators. The successful methods ($z = 0$) reduce the noise because they cut off the contribution of the high k modes in $C_r(0)$.

3. SIGNAL-TO-NOISE RATIO FOR HADRONS

The case of hadrons is quite different than that of glueballs. Power counting arguments like those leading to Table 1 predict huge z's. However, using $q\bar{q}$ mesons as an example, correlation functions are not computed by

$$C_\Gamma(t) = \sum_{\vec{x}_1,\vec{x}_2}\sum_{\vec{y}_1,\vec{y}_2} f(\vec{x}_1,\vec{x}_2)g(\vec{y}_1)g(\vec{y}_2)\times \langle\bar{\psi}(\vec{x}_1,t)\Gamma\psi(\vec{x}_2,t)\bar{\psi}(\vec{y}_1,0)\Gamma\psi(\vec{y}_2,0)\rangle \qquad (3.1)$$

where the quark bilinears, with smearing $g(\vec{y})$ and $f(\vec{x}_1,\vec{x}_2)$ at the source and sink, correspond to operators Φ_r in eq. (2.1). Instead, quark propagators $G(\vec{x},t;\vec{y},0)$ provide a much better estimate:

$$C_\Gamma(t) = \sum_{\vec{x}_1,\vec{x}_2}\sum_{\vec{y}_1,\vec{y}_2} f(\vec{x}_1,\vec{x}_2)g(\vec{y}_1)g(\vec{y}_2)\times \langle\mathrm{tr}[\Gamma G(\vec{x}_1,t;\vec{y}_1,0)\Gamma G^\dagger(\vec{x}_2,t;\vec{y}_2,0)]\rangle. \qquad (3.2)$$

The noise of eq. (3.2) is a $q\bar{q}q\bar{q}$ correlation function:

$$\sigma^2_\Gamma(t_1,t_2) = \left\langle\left(\sum_{\vec{x}_1,\vec{x}_2}\sum_{\vec{y}_1,\vec{y}_2} f(\vec{x}_1,\vec{x}_2)g(\vec{y}_1)g(\vec{y}_2)\times \mathrm{tr}[\Gamma G(\vec{x}_1,t;\vec{y}_1,0)\Gamma G^\dagger(\vec{x}_2,t;\vec{y}_2,0)]\right)^2\right\rangle - C_\Gamma(t_1)C_\Gamma(t_2) \qquad (3.3)$$

Similarly, the noise of a baryon correlation function is given by a $q\bar{q}q\bar{q}q\bar{q}$ correlation function (for SU(3)).

The lowest lying states contributing to these correlation functions will be a two (three) pion state for mesons (baryons). For t_1 and t_2 large enough for clustering

$$\sigma^2_\Gamma(t_1,t_2) \propto \exp(-M|t_1-t_2| - n_q m_\pi t_{\mathrm{min}}), \qquad (3.4)$$

where M is the mass of lowest-lying state in the channel under consideration, $n_q = 2$ ($n_q = 3$) for mesons (baryons), m_π is the mass of the (lattice) pion, and $t_{\mathrm{min}} = \min(t_1,t_2)$. Hence the signal-to-noise ratio is

$$\frac{\mathrm{SIGNAL}}{\mathrm{NOISE}} = \sqrt{N_{\mathrm{conf}}}\frac{C_\Gamma(t)}{\sigma_\Gamma(t,t)} \propto \frac{\exp(-Mt)}{\exp(-n_q m_\pi t/2)}. \qquad (3.5)$$

In this case, the relative errors increase with t, a situation that worsens in the chiral limit $m_\pi \to 0$. (In the chiral limit the error bars are t independent, like for glueballs, because $e^{-m_\pi t}$ goes over to a power law.)

The signal-to-noise ratio for hadrons can be improved by judicious choice of the smearing functions $g(\vec{y})$ and $f(\vec{x}_1,\vec{x}_2)$. A better operator is one where $\Phi_\Gamma = \sum_{\vec{x}_1,\vec{x}_2} f(\vec{x}_1,\vec{x}_2)\bar{\psi}(\vec{x}_1,t)\Gamma\psi(\vec{x}_2,t)$ has a large overlap with one-meson states, but Φ^2_Γ has almost no overlap with two-pion states.

4. EXCITED STATES

When N operators are available one can determine the matrix correlation function

$$C^{(ij)}_r(t) = \langle\Phi^{(i)}_r(t)\Phi^{(j)}_r(0)\rangle, \qquad (4.1)$$

where $i = 1,\ldots,N$ labels the operators. For example, i can denote the smearing time, the number of fuzzing

steps, or μ in the two-dimensional inverse Dirac operator. From the transfer matrix formalism

$$C_r^{(ij)}(t) = \sum_{n=1}^{M} a_n^{(i)} a_n^{(j)} e^{-m_{n,r}t} = \sum_{n=1}^{M} \hat{a}_n^{(i)}(t)\hat{a}_n^{(j)}(t), \quad (4.2)$$

where M is an number with order of magnitude N_S^3. At $\tau \sim m_{1,r}^{-1}$ one should not expect $C_r^{(ij)}(\tau)$ to contain that much information, because the higher mass states will be obscured by the noise. If the practical value of M is less than N, then $N - M$ eigenvalues of the matrix $C_r^{(ij)}(\tau)$ will be zero, and M of them will be positive. Let

$$C_r^{(ij)}(\tau) = \sum_{n=1}^{M} \lambda_n v_n^{(i)} v_n^{(j)}, \quad (4.3)$$

where $v_n^{(i)}$ is the eigenvector with eigenvalue λ_n:

$$\sum_{j=1}^{N} C_r^{(ij)}(\tau) v_n^{(j)} = \lambda_n v_n^{(i)}. \quad (4.4)$$

Together eqs. (4.2), (4.3) and the assumption $M < N$ imply

$$\hat{a}_n^{(i)}(\tau) = \sum_{m=1}^{M} R_{nm} b_m^{(i)}, \quad b_n^{(i)} = \sqrt{\lambda_n} v_n^{(i)} \quad (4.5)$$

where R_{nm} is an $M \times M$ rotation matrix. Now consider

$$z_n^{(i)} = \sum_{m=1}^{M} R_{nm} w_m^{(i)}, \quad w_n^{(i)} = v_n^{(i)}/\sqrt{\lambda_n}. \quad (4.6)$$

Then two lines of algebra show

$$\sum_{i=1}^{N} z_n^{(i)} \hat{a}_m^{(i)} = \delta_{nm}, \quad (4.7)$$

i.e. $z_n^{(i)}$ projects out the n-th state!

The number of accessible states M should be computed from the data, in the sense of singular-value decomposition.[12] After computing the eigenvalues of $C_r^{(ij)}(\tau)$ one will find a some eigenvalues of reasonable magnitude—within a factor of the relative error from the largest eigenvalue—and the others smaller still. For poor data some eigenvalues may even be negative. The number with reasonable magnitudes will be M, and the other modes will be ignored entirely:

$$\left.\begin{array}{l} \lambda_n \equiv 0 \\ \lambda_n^{-1} \equiv 0 \end{array}\right\} n > M. \quad (4.8)$$

(The second prescription is appropriate, say, for defining $w_n^{(i)}$.) Eq. (4.8) also weeds out redundant information in $C_r^{(ij)}(\tau)$ arising from similarities in the chosen operators.

The matrix R_{nm} is determined by the usual variational calculation criterion of maximizing $C_{1,r}(t)$, for some $t > \tau$, where $C_{n,r}(t) = \sum_{i,j=1}^{N} z_n^{(i)} C_r^{(ij)}(t) z_n^{(i)}$ (The normalization of $w_n^{(i)}$ is such that $C_{n,r}(\tau) = 1$. Further variations and orthogonality determine $z_n^{(i)}$ for $2 \le n \le M$. Then $m_{n,r}$ is determined by a fit to $C_{n,r}(t)$.

The refinement is that the variation is over $M - 1$ rather than $N - 1$ parameters. Whereas N is subjectively chosen, M is objectively chosen by the data.

In meson and hadron calculations the expense of computing the quark propagator likely means $N_{\mathrm{sink}} > N_{\mathrm{source}}$. As long as $N_{\mathrm{sink}}, N_{\mathrm{source}} > M$ singular value decomposition of non-square matrices follows through much as above.

An additional modification is appropriate for the channel with vacuum quantum numbers. Usually masses are computed from the connected correlation function

$$C_{r,\mathrm{c}}(t) = \langle \Phi_r(t)\, \Phi_r(0) \rangle - \langle \Phi_r \rangle \langle \Phi_r \rangle, \quad (4.9)$$

but if $\langle \Phi_r \rangle$ entails an average over t, the estimate is biased.[13] To avoid bias one can fit to the disconnected correlation function $C_{r,\mathrm{d}}(t) = \langle \Phi_r(t)\Phi_r(0) \rangle$:

$$\begin{array}{l} C_{r,\mathrm{d}}(t) = A\left(e^{-mt} + e^{-m(T-t)}\right) + B^2 \\ \langle \Phi_r \rangle = B, \end{array} \quad (4.10)$$

taking the covariance matrix of $C_{r,\mathrm{d}}(t)$ and $\langle \Phi_r \rangle$ into account. Unfortunately, unless B is small ($B^2 \lesssim A$) it is impossible to get reasonable estimates of A and m.

The variational calculation can be extended to make eq. (4.10) a viable strategy. After computing R_{nm} from $C_{r,\mathrm{c}}^{(ij)}(t)$ as above, one has, via eq. (4.5) an estimate of the $\hat{a}_n^{(i)}(\tau)$. Then define $\hat{a}_0^{(i)} = \langle \Phi_r^{(i)} \rangle$ and construct

$$\tilde{z}_n^i = \frac{1}{\mathcal{N}} \left(z_n^i - \sum_{m \neq n} \alpha_m^{(i)} \hat{a}_m^{(i)}(\tau) \right), \quad (4.11)$$

with $\mathcal{N}$ and the $\alpha_m^{(i)}$ such that $\sum_{i=1}^{N} \tilde{z}_n^{(i)} \hat{a}_m^{(i)}(\tau) = \delta_{nm}$.

4.1. A test

This variation on the variational calculation has been tested for glueballs using two-dimensional inverse Dirac matrices as operators, $\Phi^{(i)} = \mathrm{Tr}\{\mu^{(i)}/(\mathcal{D}_2 + \mu^{(i)})\}$, and $N = 20$ choices of $\mu^{(i)}$. The results from this 16^4 $\beta = 6.0$ data are in Table 2, along with results of a previous analysis,[14] which was a traditional variational calculation, minimizing the *error* in the correlation function for $t \sim m_{1,r}^{-1}$. The discrepencies in the masses are likely more due to the present reliance on the covariance

Table 2: Comparison of masses from the modified variational technique and those determined previously[14] ("old mass") from the same data.

state	mass	old mass	χ^2/dof	$t_1;t_2$	λ_1/λ_2
A_1^{++}	0.77(6)	0.67(3)	2.83/4	2;3	
	1.54(70)	–	2.08/3	3;4	4
E^{++}	1.32(8)	1.10(7)	1.02/3	2;4	65
e_1	0.864(41)	0.876(30)	1.61/3	2;5	170

matrix[15] between time-slices than the new variational estimate. (The old analysis did not take the covariance matrix into account.) Fits to excited states were done with fixed lowest-lying mass and variable lowest-lying amplitude. In all cases (including those not tabulated because of unreliable error estimates) the lowest-lying amplitude was consistent with zero.

The results of the test are disappointing. Only for A_1^{++} was the eigenvalue ratio λ_1/λ_2 small enough to obtain a reasonable estimate. In addition to the obvious problem that high-mass states ($ma > 1$) decay out of the correlation function in a few timeslices, the operators chosen were probably not linearly independent enough to resolve differences between excited states and the ground state. This may also explain the Ape result that the excited states were consistent with n-glueball states.[5]

5. MOMENTUM-SPACE OPERATORS

Recall that the vector $z_n^{(i)}$ has the interpretation of a wave function projected onto the space spanned by $\Phi^{(i)}|0\rangle$. If lack of linear independence in these basis states hinders the variational computation, one should seek a more independent set. It seems unlikely that presently established methods are versatile enough to tune them in the necessary way. A possibility is to use gauge-fixed momentum-space operators, that is, operators built out of gauge potentials $A_\mu(p)$ and quark fields $\psi(p)$. As long as the momentum p is not ultraviolet, power counting[8] argues that glueballs will not have a critical signal-to-noise problem. It is also quite easy to construct operators. For example, $\Phi_{\mu\nu}^{(i)} = A_\mu(p^{(i)})A_\nu(-p^{(i)})$, $\mu,\nu \in \{1,2,3\}$, couples to A_1^{++}, E^{++}, T_2^{++} and T_1^{-+}. One might also hope that it is possible to construct hadron operators $\Phi_\Gamma^{(i)}$ whose square does not couple much to pions.

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